

# Non-Markovian dynamics for an open two-level system without rotating wave approximation: Indivisibility versus backflow of information

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## Abstract

By use of the two measures presented recently, the indivisibility and the backflow of information, we study the non-Markovianity of the dynamics for a two-level system interacting with a zero-temperature structured environment without using rotating wave approximation (RWA). In the limit of weak coupling between the system and the reservoir, and by expanding the time-convolutionless (TCL) generator to the forth order with respect to the coupling strength, the time-local non-Markovian master equation for the reduced state of the system is derived. Under the secular approximation, the exact analytic solution is obtained and the sufficient and necessary conditions for the indivisibility and the backflow of information for the system dynamics are presented. In the more general case, we investigate numerically the properties of the two measures for the case of Lorentzian reservoir. Our results show the importance of the counter-rotating terms to the short-time-scale non-Markovian behavior of the system dynamics, further expose the relations between the two measures and their rationality as non-Markovian measures. Finally, the complete positivity of the dynamics of the considered system is discussed.

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## I. INTRODUCTION

Realistic quantum systems cannot avoid interactions with their environments, thus the study of open quantum systems is very important. It is not only relevant for better understanding of quantum theory, but also fundamental for various modern applications of quantum mechanics, especially for quantum communication, cryptography and computation [1]. The early study of dynamics of open quantum systems usually consists in the application of an appropriate Born-Markov approximation, that is, neglects all the memory effects, leading to a master equation which can be cast in the so-called Lindblad form [2, 3]. Master equations in Lindblad form can be characterized by the fact that the dynamics of the system satisfies both the semigroup property and the complete positivity, thus ensuring the preservation of positivity of the density matrix during the time evolution. We usually attribute the dynamical processes with these evolutionary properties to the well-known Markovian ones.

However, people recently found that Many relevant physical systems, such as the quantum optical system [4], quantum dot [5], superconductor system [6], could not be described simply by Markovian dynamics. Similarly, quantum chemistry [7] and the excitation transfer of a biological system [8] also need to be treated as non-Markovian processes. Quantum non-Markovian processes can lead to distinctly different effects on decoherence and disentanglement [9, 10] of open systems compared to Markovian processes. These non-markovian effects can on the one hand enrich the basic theory of quantum mechanics, on the other hand benefit the quantum information processing. Because of these distinctive properties and extensive applications, more and more attention and interest have been devoted to the study of non-Markovian processes of open systems, including the measures of non-Markovianity [11–19], the positivity [20–22], and some other dynamical properties [23–27] and approaches [28–30] of non-Markovian processes. Experimentally, the simulation [31, 32] of non-Markovian environment has been realized.

The measure of non-Markovianity of quantum evolution is a fundamental problem which aims to detect whether a quantum process is non-Markovian and how much degrees it deviates from a Markovian one. Based on the distinguishability of quantum states, Breuer, Laine and Piilo (BLP) [11] proposed a measure to detect the non-Markovianity of quantum processes which is linked to the flow of information between the system and environ-

ment. Alternatively, Rivas, Huelga and Plenio [13] (RHP) also presented a measure of non-Markovianity by employing the dynamical divisibility of a trace-preserving completely positive map. It is clear that the BLP measure is based on the physical features of the system-reservoir interactions, while the RHP definition is based on the mathematical property of the dynamical maps. It has been shown that the two measures agree for several important and commonly-used models [33], but do not agree in general [34]. In this paper, we will use both the two measures to describe the non-Markovianity of the dynamics of the considered system, so as to more clearly see their relation, as well as the rationality as the measure of non-Markovianity.

The study of the dynamics of non-Markovian open quantum systems is typically very involved and often requires some approximations. Almost all the previous treatments are based on the RWA, that is, neglect the counter-rotating terms in the microscopic system-reservoir interaction Hamiltonian. However, the counter-rotating terms which are responsible for the virtual exchanges of energy between the system and the environment not always can be neglected. For example, for the wide-frequency-spectra reservoir or when the frequency distribution of the structured environment is detuned large enough from the transition of the system, the RWA is invalid. Another motivation of this paper is thus to study the effect of the counter-rotating terms on the non-Markovian dynamics of the considered open quantum system.

The article is organized as follows. In Sec. II we introduce the microscopic Hamiltonian model between the system and its environment, and derive the non-Markovian time-local master equation for a two-level system weakly coupled to a vacuum reservoir, by using the TCL approach to the forth-order but without employing RWA in the interaction Hamiltonian. In Sec. III, we investigate the non-Markovianity of the system dynamics in terms of both the RHP and BLP measures. Through the analytical solution in the secular approximation, we obtain the sufficient and necessary conditions for the dynamical indivisibility and the backflow of information, showing the effect of the counter-rotating terms on the non-Markovian dynamics of the system, and exposing the relations between the BLP and RHP measures. In sec. IV, by choosing the Lorentzian spectra reservoir as an exemplary example, we further demonstrate the effect of the counter-rotating terms on the dynamical indivisibility and the backflow of information, and clarify the rationality of the two non-Markovian measures. Finally in Sec.V, we discuss simply the complete positivity of the

system dynamics. And the conclusion is arranged in Sec.VI.

## II. THE MICROSCOPIC MODEL

Consider a two-level atom with Bohr frequency  $\omega_0$  interacting with a zero-temperature bosonic reservoir modeled by an infinite chain of quantum harmonic oscillators. The total Hamiltonian for this system in the Schrödinger picture is given by

$$H = \frac{1}{2}\omega_0\sigma_z + \sum_k \omega_k b_k^\dagger b_k + \sum_k g_k(\sigma_+ + \sigma_-)(b_k + b_k^\dagger), \quad (1)$$

where  $\sigma_z$  and  $\sigma_\pm$  are the Pauli and inversion operators of the atom,  $\omega_k$ ,  $b_k$  and  $b_k^\dagger$  are respectively the frequency, annihilation and creation operators for the  $k$ -th harmonic oscillator of the reservoir. The coupling strength  $g_k$  is assumed to be real for simplicity. The distinct feature of this Hamiltonian is the reservation of the counter-rotating terms,  $\sigma_+ b_k^\dagger$  and  $\sigma_- b_k$ , which is the so-called without RWA we call in this paper. Note however that our starting point is the dipole interaction Hamiltonian between the atom and its environment, whose derivation starting with the canonical Hamiltonian involves the discarding of a term which is quadratic with respect to the radiation field. The discarding is not based on the RWA, but the fact that for low-intensity radiation, the quadratic term is much small compared to the dipole interaction one [36].

The time-convolutionless projection operator technique is most effective in dealing with the dynamics of open quantum systems. In the limit of weak coupling between the system and the environment, by expanding the TCL generator to the forth order with respect to coupling strength, the non-Markovian master equation describing the evolution of the reduced system, in the interaction picture, can be written as [For the main clue of its derivation, see appendix A.]

$$\frac{d\rho(t)}{dt} = -i[H_{LS}(t), \rho(t)] + D[\rho(t)] + D'[\rho(t)], \quad (2)$$

where

$$H_{LS}(t) = S_+(t)\sigma_+\sigma_- + S_-(t)\sigma_-\sigma_+, \quad (3)$$

is the Lamb shift Hamiltonian which describes a small shift in the energy of the eigenstates of the two-level atom. In many theoretical researches [23], this term was neglected usually.

But in this paper, we will take it into the consideration. The Lamb shift includes the second and forth order contributions,

$$S_{\pm}(t) = S_{\pm}^{II}(t) + S_{\pm}^{IV}(t), \quad (4)$$

which respectively come from the second and forth order perturbative expansion of the TCL generator. The second order Lamb shift is

$$S_{\pm}^{II}(t) = \pm \int_0^t d\tau \int d\omega J(\omega) \sin[(\omega_0 \mp \omega)\tau], \quad (5)$$

with  $J(\omega) = \sum_k |g_k|^2 \delta(\omega - \omega_k)$  the spectral distribution of the environment. The expression for the forth order Lamb shift  $S_{\pm}^{IV}(t)$  is cumbersome which is presented in the appendix A.

The dissipator  $D[\rho(t)]$  that describes the secular motion of the system has the form

$$\begin{aligned} D[\rho(t)] = & \Gamma_{-}(t) \{ \sigma_{-} \rho(t) \sigma_{+} - \frac{1}{2} \{ \sigma_{+} \sigma_{-}, \rho(t) \} \} \\ & + \Gamma_{+}(t) \{ \sigma_{+} \rho(t) \sigma_{-} - \frac{1}{2} \{ \sigma_{-} \sigma_{+}, \rho(t) \} \} \\ & + \Gamma_0(t) \{ \sigma_{+} \sigma_{-} \rho(t) \sigma_{+} \sigma_{-} - \frac{1}{2} \{ \sigma_{+} \sigma_{-}, \rho(t) \} \}, \end{aligned} \quad (6)$$

where the first line describes the dissipation of the atom to the vacuum environment with time-dependent decay rate  $\Gamma_{-}(t)$ , and the second line denotes the heating of the atom in the vacuum environment with time-dependent heating rate  $\Gamma_{+}(t)$ . This heating is related to the dissipation, for a ground-state atom in a zero-temperature environment, there is no heating effect. Dissipation and heating are usually accompanied by decoherence. The last line in eq.(6) describes the pure decoherence with time-dependent decoherence rate  $\Gamma_0(t)$ . The time-dependent transition rates  $\Gamma_{\pm}(t)$  also include the second and forth order perturbative contributions of the TCL generator,

$$\Gamma_{\pm}(t) = \Gamma_{\pm}^{II}(t) + \Gamma_{\pm}^{IV}(t), \quad (7)$$

with the second order contribution as

$$\Gamma_{\pm}^{II}(t) = 2 \int_0^t d\tau \int d\omega J(\omega) \cos[(\omega_0 \pm \omega)\tau]. \quad (8)$$

While  $\Gamma_0(t)$  completely comes from the forth-order perturbative contribution. All the forth-order contributions are presented in the appendix A. Eq.(6) indicates that the dissipative model of eq.(1), except for inducing the energy exchange between the system and its environment, also makes decoherence of the system. But the rate of decoherence is much less

than that of energy dissipation, because  $\Gamma_0(t)$  is only a forth-order contribution term of TCL perturbative expansion.

The dissipator  $D'[\rho(t)]$  represents the contribution of the so-called nonsecular terms, that is, terms oscillating rapidly with Bohr frequency  $\omega_0$ ,

$$D'[\rho(t)] = [\alpha(t) + i\beta(t)]\sigma_+\rho(t)\sigma_+ + h.c., \quad (9)$$

here  $h.c.$  denotes the Hermitian conjugation. These nonsecular terms sometimes may also be neglected under the so-called secular approximation [35]. The time-dependent coefficients  $\alpha(t)$  and  $\beta(t)$  also include the second and forth order contributions,

$$\alpha(t) = \alpha^{II}(t) + \alpha^{IV}(t), \quad (10)$$

$$\beta(t) = \beta^{II}(t) + \beta^{IV}(t), \quad (11)$$

with

$$\alpha^{II}(t) = 2 \int_0^t d\tau \int d\omega J(\omega) \cos[\omega(t - \tau)] \cos[\omega_0(t + \tau)], \quad (12)$$

and

$$\beta^{II}(t) = 2 \int_0^t d\tau \int d\omega J(\omega) \cos[\omega(t - \tau)] \sin[\omega_0(t + \tau)]. \quad (13)$$

The forth-order contributions are listed in the appendix A.

Note that the dynamics for a two-level system embedded in a zero-temperature structured environment, under RWA, can be solved exactly, where the corresponding master equation has the Lindblad-like form [4],

$$\frac{d}{dt}\rho(t) = -\frac{i}{2}S(t)[\sigma_+\sigma_-, \rho(t)] + \gamma(t)\{\sigma_-\rho(t)\sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-, \rho(t)\}\}, \quad (14)$$

where the time-dependent decay rate  $\gamma(t)$  and Lamb shift  $S(t)$  are related to the correlation function of the reservoir. Comparing this equation with eq.(2), we see that the last two terms in the dissipator  $D[\rho(t)]$ , that is, the heating and the pure decoherence terms, as well as the nonsecular dissipator  $D'[\rho(t)]$  and the Lamb shift  $S_-(t)$ , are completely from the contribution of the counter-rotating terms presented in the interaction Hamiltonian. While the decay rate  $\Gamma_-(t)$  and the Lamb shift  $S_+(t)$  include the contributions of both rotating and counter-rotating terms, but the main contributions [i.e., the second-order terms  $\Gamma_-^{II}(t)$  and  $S_+^{II}(t)$ ] come from the rotating terms. In fact, by expanding the decay rate  $\gamma(t)$  and the Lamb shift  $S(t)$  to the second order with respect to coupling strength, one obtain  $\Gamma_-^{II}(t)$

and  $S_+^{II}(t)$  [4]. In the following, we will show that the contributions that come from the counter-rotating terms are important, in particular to the short-time-scale non-Markovian behaviors.

### III. MEASURES OF NON-MARKOVIANITY

Recently, people have been interested in the study of non-Markovianity of open quantum systems. Several definitions or measures [11, 13–16] of non-Markovian dynamics have been presented. In this section, we will employ two of the measures, i.e., the RHP [13] and BLP [11] measures, to investigate the non-Markovian dynamics of the considered system so as to see the effect of the counter-rotating terms on non-Markovianity and the relation between the two measures.

#### A. Divisible and indivisible dynamics

A trace-preserving completely positive map  $\varepsilon(t_2, 0)$  that describes the evolution from times zero to  $t_2$  is divisible if it satisfies composition law,

$$\varepsilon(t_2, 0) = \varepsilon(t_2, t_1)\varepsilon(t_1, 0), \quad (15)$$

with  $\varepsilon(t_2, t_1)$  being completely positive for any  $t_2 \geq t_1 \geq 0$ . Due to the continuity of time, eq.(15) is always fulfilled in form. The key point for divisibility is actually the complete positivity of  $\varepsilon(t_2, t_1)$  for any  $t_2 \geq t_1 \geq 0$ . If there exist times  $t_1$  and  $t_2$  such that the map  $\varepsilon(t_2, t_1)$  is not completely positive, then the dynamical map  $\varepsilon(t_2, 0)$  is indivisible. RHP [13] defined all the divisible maps to be Markovian. Therefore, the indivisibility of a map advocates its dynamical non-Markovianity. It was shown that all the evolutions governed by Lindblad-type master equation with positive transition rates are divisible [37], thus Markovian.

It was proved [13] that the indivisibility of map  $\varepsilon(t, 0)$  is equivalent to the complete positivity of the quantity,

$$g(t) = \lim_{\epsilon \rightarrow 0^+} \frac{\|[\varepsilon(t + \epsilon, t) \otimes I]|\Phi\rangle\langle\Phi|\| - 1}{\epsilon}. \quad (16)$$

Only for divisible map,  $g(t) = 0$ . Where  $|\Phi\rangle$  is a maximally entangled state between the system of interest and an ancillary particle, and the map  $\varepsilon$  performs only on the state

of the system. Using the time-local master equation  $\frac{d\rho}{dt} = \mathcal{L}_t(\rho)$ , this expression may be equivalently written as [13]

$$g(t) = \lim_{\epsilon \rightarrow 0^+} \frac{\|[I + (\mathcal{L}_t \otimes I)\epsilon]|\Phi\rangle\langle\Phi|\| - 1}{\epsilon}. \quad (17)$$

The function  $g(t)$  is the so-called RHP non-Markovian measure. If and only if  $g(t) = 0$  for every time  $t \in \{0, t_2\}$ , the map  $\varepsilon(t_2, 0)$  is Markovian. Otherwise it is non-Markovian. The distinctive advantage of RHP non-Markovian measure is that its calculation can be processed only by the use of time-local master equation, not requiring the exact form of the dynamical map  $\varepsilon(t, 0)$ . In the following, we call the time interval that satisfies  $g(t) > 0$  the indivisible dynamical interval (IDI). For a non-Markovian process, there must exist one or several IDIs.

For the open two-level system considered in this paper, suppose that  $|\Phi\rangle = \frac{1}{\sqrt{2}}[|01\rangle + |10\rangle]$ , a straightforward deduction using equations (2) and (17) gives

$$\begin{aligned} g = & \frac{1}{4}|\Gamma_- + \Gamma_+ + \sqrt{(\Gamma_- - \Gamma_+)^2 + 4(\alpha^2 + \beta^2)}| \\ & + \frac{1}{4}|\Gamma_- + \Gamma_+ - \sqrt{(\Gamma_- - \Gamma_+)^2 + 4(\alpha^2 + \beta^2)}| \\ & + \frac{1}{4}[|\Gamma_0| - \Gamma_0 - 2\Gamma_- - 2\Gamma_+], \end{aligned} \quad (18)$$

where for compactness we omit the argument of all the time-dependent coefficients. Obviously, the Lamb shift  $H_{LS}(t)$  has no effect on the indivisibility of the system dynamics.

## B. Backflow of information

The second measure of non-Markovianity for quantum processes of open systems we employ is proposed by BLP [11] which is based on the consideration in purely physics. Note that Markovian processes always tend to continuously reduce the trace distance between any two states of a quantum system, thus an increase of the trace distance during any time interval implies the emergence of non-Markovianity. BLP further linked the change of the trace distance to the flow of information between the system and its environment, and concluded that the back flow of information from environment to the system is the key feature of a non-Markovian dynamics. In quantum information science, the trace distance



for quantum states  $\rho_1$  and  $\rho_2$  is defined as [1]

$$D(\rho_1, \rho_2) = \frac{1}{2} \text{tr} |\rho_1 - \rho_2|, \quad (19)$$

with  $|A| = \sqrt{A^\dagger A}$ . For a given pair of initial states  $\rho_{1,2}(0)$  of the system, the change of the dynamical trace-distance can be described by its time derivative

$$\sigma(t, \rho_{1,2}(0)) = \frac{d}{dt} D(\rho_1(t), \rho_2(t)), \quad (20)$$

where  $\rho_{1,2}(t)$  are the dynamical states of the system with the initial states  $\rho_{1,2}(0)$ . For Markovian processes, the monotonically reduction of the trace distance implies  $\sigma(t, \rho_{1,2}(0)) \leq 0$  for any initial states  $\rho_{1,2}(0)$  and at any time  $t$ . If there exists a pair of initial states of the system such that for some evolutionary time  $t$ ,  $\sigma(t, \rho_{1,2}(0)) > 0$ , then the information takes backflow from environment to the system, and the process is non-Markovian.

In order to calculate the BLP measure, we must solve the dynamics of the system. For this purpose, we write the alternative Bloch equation of eq.(2) as [see appendix B for their derivation],

$$\dot{b}_x = -\frac{1}{2}(\Gamma_- + \Gamma_+ + \Gamma_0 - 2\alpha)b_x + (S_- - S_+ - \beta)b_y, \quad (21)$$

$$\dot{b}_y = -\frac{1}{2}(\Gamma_- + \Gamma_+ + \Gamma_0 + 2\alpha)b_y - (S_- - S_+ + \beta)b_x, \quad (22)$$

$$\dot{b}_z = -(\Gamma_- + \Gamma_+)b_z + \Gamma_+ - \Gamma_-, \quad (23)$$

where the three components of the Bloch vector are defined as  $b_j(t) = \text{Tr}[\rho(t)\sigma_j]$  with  $j = x, y, z$  and  $\sigma_j$  the Pauli operators. In terms of Bloch vector, the trace distance of eq.(19) may be expressed as

$$D(t) = \frac{1}{2} \sqrt{(\Delta b_x)^2 + (\Delta b_y)^2 + (\Delta b_z)^2} \quad (24)$$

where  $\Delta b_j = b_{1j}(t) - b_{2j}(t)$  are the differences between the two Bloch components at evolutionary time  $t$ . Correspondingly, the derivative of this trace distance becomes

$$\begin{aligned} \sigma = & -\frac{1}{4} [(\Delta b_x)^2 + (\Delta b_y)^2 + (\Delta b_z)^2]^{-1/2} \{ (\Gamma_- + \Gamma_+ + \Gamma_0 - 2\alpha)(\Delta b_x)^2 \\ & + (\Gamma_- + \Gamma_+ + \Gamma_0 + 2\alpha)(\Delta b_y)^2 + 4\beta(\Delta b_x)(\Delta b_y) + 2(\Gamma_- - \Gamma_+)(\Delta b_z)^2 \}, \end{aligned} \quad (25)$$

where we have used the Bloch eqs.(21)-(23) in the deduction process. According BLP's criterion,  $\sigma > 0$  indicates the backflow of information from environment to the system. In the following, we call the time intervals in which  $\sigma(t) > 0$  the information-backflow intervals (IBIs).

### C. Secular approximation

In order to see the effect of counter-rotating terms and make a distinct comparison between the BLP and RHP measures in the current system, we now consider the case where the nonsecular term  $D'[\rho(t)]$  can be neglected, i.e., performing the so-called secular approximation. Here for the sake of discrimination, we call as in many literatures *the rotating-wave approximation that used after tracing over the bath degrees of freedom* the secular approximation. In other words, the secular approximation and the RWA have the same mathematical approaches—throwing away the rapidly oscillating terms in time, merely the times the approximations taking place are different. Just as pointed out in reference [35], this kind of secular approximation though also is an average over rapidly oscillating terms, it does not wash out the effect of the counter-rotating terms present in the coupling Hamiltonian. Under the secular approximation, the master equation (2) has the Lindblad-like form with time-dependent transition rates,  $\Gamma_{\pm}(t)$ ,  $\Gamma_0(t)$  and Lamb shift  $H_{LS}(t)$ . Employing the method proposed in [39], the corresponding Bloch eqs.(21)-(23) in this case can be solved exactly which gives

$$b_x(t) = e^{-\Theta(t)}[b_x(0) \cos \delta(t) - b_y(0) \sin \delta(t)], \quad (26)$$

$$b_y(t) = e^{-\Theta(t)}[b_x(0) \sin \delta(t) + b_y(0) \cos \delta(t)], \quad (27)$$

$$b_z(t) = e^{-\Lambda(t)} \left\{ b_z(0) + \int_0^t ds e^{\Lambda(s)} [\Gamma_+(s) - \Gamma_-(s)] \right\}, \quad (28)$$

with

$$\Theta(t) = \frac{1}{2} \int_0^t ds [\Gamma_-(s) + \Gamma_+(s) + \Gamma_0(s)], \quad (29)$$

$$\Lambda(t) = \int_0^t ds [\Gamma_-(s) + \Gamma_+(s)], \quad (30)$$

and

$$\delta(t) = \int_0^t ds [S_+(s) - S_-(s)]. \quad (31)$$

Inserting these solutions into eq.(25), we get

$$\begin{aligned} \sigma = & -\frac{1}{4} I(t) \{ e^{-2\Theta(t)} (\Gamma_- + \Gamma_+ + \Gamma_0) [(\Delta b_x(0))^2 + (\Delta b_y(0))^2] \\ & + 2e^{-2\Lambda(t)} (\Gamma_- + \Gamma_+) (\Delta b_z(0))^2 \}, \end{aligned} \quad (32)$$

where  $I(t) = \{ e^{-2\Theta(t)} [(\Delta b_x(0))^2 + (\Delta b_y(0))^2] + e^{-2\Lambda(t)} (\Delta b_z(0))^2 \}^{-1/2}$  is a positive function and  $\Delta b_j(0) = b_{1j}(0) - b_{2j}(0)$  is the difference between the two initial Bloch components. This

expression shows that the sufficient and necessary conditions for the backflow of information from environment to the system are

$$\Gamma_{-}(t) + \Gamma_{+}(t) + \Gamma_0(t) < 0, \quad (33)$$

or

$$\Gamma_{-}(t) + \Gamma_{+}(t) < 0. \quad (34)$$

Because if at some time  $t$ , one of this conditions is satisfied, then we can always find a pair of initial states such that  $\sigma(t) > 0$ . For example, if eq.(33) fulfils, it suffices to choose the initial states satisfying  $\Delta b_z(0) = 0$ . Conversely, if  $\sigma(t) > 0$  at some time  $t$ , then at least one of the two conditions must be satisfied.

On the other hand, under secular approximation, eq.(18) is simplified as

$$g = \frac{1}{4}\{2|\Gamma_{-}| + 2|\Gamma_{+}| + |\Gamma_0| - 2\Gamma_{-} - 2\Gamma_{+} - \Gamma_0\}. \quad (35)$$

Obviously, when one of the three rate functions,  $\Gamma_{-}(t)$ ,  $\Gamma_{+}(t)$  or  $\Gamma_0(t)$ , is negative, then  $g > 0$ , vice versa. Thus the sufficient and necessary conditions for the indivisibility of the dynamics are

$$\Gamma_{-}(t) < 0, \text{ or } \Gamma_{+}(t) < 0, \text{ or } \Gamma_0(t) < 0. \quad (36)$$

Eqs. (33), (34) and (36) demonstrate two important results. One the one hand, the counter-rotating terms [which induce  $\Gamma_{+}(t)$ ,  $\Gamma_0(t)$  and a part of  $\Gamma_{-}^{IV}(t)$ ] may have important effect to the non-Markovian dynamics of the system, according to RHP and BLP measures. On the other hand, they show that the conditions for the backflow of information are much more rigorous than that of indivisibility. The later only requires one of the transition rates to be negative, while the former further requires the sum of the two or the total transition rates to be negative. This conditionality once again validates the previous results: The backflow of information must lead the indivisibility of the dynamics, but the reverse is not true [34]. However, for Lindblad-like master equation with only single transition rate, the sufficient and necessary conditions for the two measures become clearly the same, denoting the consistency of the two measures in this case [33].

#### IV. NON-MARKOVIAN DYNAMICS FOR LORENTZIAN SPECTRUM

In order to further demonstrate quantitatively the effect of the counter-rotating terms, as well as the rationality of the two non-Markovian measures, we specify our study to a

particular reservoir spectra, Lorentzian spectra,

$$J(\omega) = \frac{\gamma_0 \lambda^2}{2\pi[(\omega_0 - \omega - \Delta)^2 + \lambda^2]}, \quad (37)$$

which describes the interaction of an atom with an imperfect cavity and is widely used in literatures. Where  $\omega_0$  denotes the transition frequency of the atom,  $\Delta = \omega_0 - \omega_c$  is the frequency detuning between the atom and the cavity mode.  $\lambda$  is the width of Lorentzian distribution, which is connected to the reservoir correlation time  $\tau_R = \lambda^{-1}$ . The parameter  $\gamma_0$  can be regarded as the decay rate for the excited atom in the Markovian limit of flat spectrum which is related to the relaxation time  $\tau_S = \gamma_0^{-1}$ . For the Lorentzian spectra, all the time-dependent coefficients including  $S_{\pm}(t)$ ,  $\Gamma_{\pm}(t)$ ,  $\Gamma_0(t)$ ,  $\alpha(t)$  and  $\beta(t)$  can be calculated analytically, but the expressions are too complicated. We thus study them only numerically.

In Fig.1, we show the time evolution of these coefficients. For our purpose, we intentionally choose three special sets of parameters. It shows that for narrow spectrum and small detuning [In Fig.1 (a) and (d),  $\lambda/\omega_0 = 0.2\%$ ,  $\Delta/\omega_0 = 2\%$ ],  $\Gamma_-(t)$  plays the dominant role, while  $\Gamma_+(t)$  and  $\Gamma_0(t)$  are almost zero. The nonsecular coefficients  $\alpha(t)$  and  $\beta(t)$  in this case behave fast oscillations [Fig.1 (d)], so that on average in time the effect can also be neglected. These results imply that for this set of parameters, the counter-rotating terms in Hamiltonian (1) play little effect actually to the system dynamics and the commonly-used RWA is valid. However, for wider spectrum or/and larger detuning, the results are different [see Fig.1 (b) and (c)], where though  $\Gamma_0$  is still near zero [38],  $\Gamma_+$  clearly can not be neglected. Thus the counter-rotating terms in these cases are important and the RWA is invalid. Of course, for very wide spectrum, one may expect that the dynamics tends to be Markovian. The positivity of the  $\Gamma_{\pm}(t)$  and  $\Gamma_0(t)$  in Fig.1 (c) confirms this point. In addition, when  $\lambda$  is small, the correlation time of the environment is longer, thus  $\Gamma_-$  in Fig.1 (a) oscillates to emerge negative values in a relatively longer time. With the increasing of  $\lambda$ , the correlation time becomes small and small, and the times for  $\Gamma_{\pm}$  to be negative shorten or even vanish [Fig.1 (b) and (c)]. Note that the observable negative values of  $\Gamma_+$  in Fig.1 (b) demonstrate the contribution of the counter-rotating terms to the non-Markovianity of the system dynamics.

Note that in the RWA, the corresponding master equation (14) may be solved exactly.

For the Lorentzian spectrum, the RHP and BLP measures may be expressed as [33],

$$g(t) = \begin{cases} 0 & \text{for } \gamma(t) \geq 0 \\ -\gamma(t) & \text{for } \gamma(t) < 0 \end{cases} \quad (38)$$

and

$$\sigma(t) = -\gamma(t)F(t). \quad (39)$$

where

$$\gamma(t) = \text{Re} \left[ \frac{2\gamma_0\lambda \sinh(dt/2)}{d \cosh(dt/2) + (\lambda - i\Delta) \sinh(dt/2)} \right], \quad (40)$$

with  $d = \sqrt{(\lambda - i\Delta)^2 - 2\gamma_0\lambda}$ . The positive real function  $F(t)$  is defined as,

$$F(t) = \frac{a^2 e^{-\frac{3}{2}\Gamma(t)} + |b|^2 e^{-\frac{1}{2}\Gamma(t)}}{\sqrt{a^2 e^{-\Gamma(t)} + |b|^2}}, \quad (41)$$

with  $\Gamma(t) = \int_0^t dt' \gamma(t')$ , and  $a = \langle 1|\rho_1(0)|1\rangle - \langle 1|\rho_2(0)|1\rangle$ ,  $b = \langle 1|\rho_1(0)|0\rangle - \langle 1|\rho_2(0)|0\rangle$  being the differences of the population and of coherence respectively for the two given initial states. Eqs.(38) and (39) show that under the RWA, the distributions of IDIs and IBIs are exactly the same, which are determined by  $\gamma(t) < 0$ . In the following, we study numerically the evolution of the measures  $\sigma$  and  $g$ , under the condition without using RWA, so as to further highlight the non-Markovian effect of the counter-rotating terms, as well as the rationality of BLP and RHP measures.

In Fig.2, we show the time evolution of the measure  $\sigma$  in the same parameters as in Fig.1, where the solid lines are plotted according to eq.(25) and the dot lines according to eq.(39). We choose the pair of initial states to be  $\rho_1(0) = |1\rangle\langle 1|$  and  $\rho_2(0) = |0\rangle\langle 0|$ , which can maximize the BLP measure [11]. For evidence, we only give the time intervals of  $\sigma > 0$ , i.e., the IBIs. We can see clearly the corrections of the counter-rotating terms on the BLP measure. In Fig.2 (a), both the distributions of the IBIs and the shapes of the two curves are similar, responding that the counter-rotating terms make lesser effect to the backflow of information in this case which is in line with the idea of RWA. The dips on each peaks of the solid-line in Fig.2 (b) are due to the negativity of  $\Gamma_+(t)$  at that times [see Fig.1 (b)], implying that  $\Gamma_+$  has the offset on the backflow of information. There is no IBI in Fig.2 (c), denoting that under the choice of this set of parameters, there is no backflow of information, or equivalently the dynamics is Markovian according to BLP measure, which is in line with the non-negativity of  $\Gamma_{\pm}(t)$  and  $\Gamma_0(t)$ . In addition, the time scale for the backflow of information

is consistent with the reservoir correlation time  $\lambda^{-1}$  [Fig.2 (a), (b)]. All these results show that on the one hand the counter-rotating terms can affect the backflow of information, and on the other hand the correction of the counter-rotating terms on the backflow of information is reasonable.

In Fig.3, we plot the time evolution of the measure  $g$  in the same parameters as in Fig.1. We see that when the counter-rotating terms are omitted, the distribution of the IDIs agrees with that of IBIs [see the dot lines in Figs. 2 and 3]. The non-Markovian time scale predicted by measure  $g$  is also in accordance with the reservoir correlation time  $\lambda^{-1}$ . The horizontal dot line in Fig.3(c) denotes that under the choice of those parameters, the dynamics is actually Markovian. All these results show that with no counter-rotating terms, the RHP and BLP measures agree. Both of them can depict rightly the non-Markovianity of the underlying dynamics. However, when the counter-rotating terms are considered, the case is distinctly different: The IDIs now become  $(0, \infty)$  [see the solid lines in Fig.3], which are clearly inconsistent with the practice. Because first of all, the non-Markovian time scales in the underlying conditions are never infinite. Next, in Fig.3(a), the choice of the parameters is consistent with the RWA, the result after considering counter-rotating terms should have some tiny, not distinct amendments, over the result under RWA. For the parameters in Fig.3(c), the reservoir correlation time  $\lambda^{-1}$  is very short and the system dynamics is actually Markovian, should not appear long-time non-Markovianity. These egregious results denote that the RHP measure in these cases is invalid. Note that the reason for resulting in these unpractical phenomena is mainly due to the nonsecular coefficients  $\alpha(t)$  and  $\beta(t)$ . When these nonsecular coefficients are neglected, eq.(35) is not seen to deviate obviously from the practice.

## V. COMPLETE POSITIVITY

The evolution of a real physical state should be not only positive but also complete positive. In practical theoretical study, however, due to the application of some assumptions and approximations, the positivity or the complete positivity may not always be satisfied. Here we present a study of the complete positivity for our considered model, i.e., the master equation of (2). As the damping matrix has the block diagonal form (see appendix B), thus we can directly use the conditions for complete positivity presented by Hall [39]. The

necessary condition of the complete positivity, for the master equation (2), may be given by two inequalities:

$$\Lambda(t) \geq 0, \quad (42)$$

$$2\Theta(t) \geq \Lambda(t), \quad (43)$$

with  $\Theta(t)$  and  $\Lambda(t)$  given by eqs.(29)-(30). The sufficient condition is also given by two inequalities. The first one coincides with eq.(42) and the second one may be expressed as

$$\chi(t) \cosh \theta(t) \leq 1 + A^2(t) - \kappa^2(t) - 2|A(t) - \chi(t)|, \quad (44)$$

where  $\chi(t) = e^{-2\Theta(t)}$ ,  $A(t) = e^{-\Lambda(t)}$ ,  $\kappa(t) = A(t) \int_0^t ds [\Gamma_+(s) - \Gamma_-(s)] A^{-1}(s)$ , and  $\theta(t) = 2 \int_0^t ds \sqrt{\alpha^2(s) + \beta^2(s)}$  with  $\alpha(t)$ ,  $\beta(t)$  given by eqs.(10)-(11). Using inequality (43) to release the modulus in the right-hand side, we get

$$\chi(t) \cosh \theta(t) \leq [1 - A(t)]^2 + 2\chi(t) - \kappa^2(t), \quad (45)$$

Note that the left-hand side of eq.(45) is relevant to the nonsecular motion, but the right-hand side only depends on the secular motion. As  $\theta(t)$  increases with time  $t$ , eq.(45) is not satisfied for long times. But in short non-Markovian time scales we are interested in, it may be fulfilled. In order to see this, we plot the time evolution of function  $G(t) \equiv [1 - A(t)]^2 + 2\chi(t) - \kappa^2(t) - \chi(t) \cosh \theta(t)$  as in Fig.4, for the same parameters as in Fig.1 and under the Lorentzian spectra. Obviously, in the scale of the correlation times  $\lambda^{-1}$ ,  $G(t) > 0$ . The condition of eqs.(42)-(43) is satisfied for all times in this case. Thus in the short non-Markovian time scales, the evolution of the system is physical. In the secular regime, the sufficient condition eq.(45) can be relaxed to

$$[1 - A(t)]^2 + \chi(t) - \kappa^2(t) \geq 0, \quad (46)$$

which can be satisfied for much more longer times for the Lorentzian reservoir.

## VI. CONCLUSION

In conclusion, we have studied the non-Markovianity of the dynamics for a two-level system interacting with a zero-temperature structured environment without using RWA. In the limit of weak coupling between the system and its reservoir, by expanding the TCL

generator to the forth order with respect to the coupling strength, we have derived the time-local non-Markovian master equation for the reduced state of the system. Under the secular approximation, the TCL master equation has the Lindblad-like form with time-dependent transition rates. We have obtained the exact analytic solution. The sufficient and necessary conditions for the indivisibility and the backflow of information for the system dynamics were presented, which showed two important results: First, the counter-rotating terms may play important roles to the indivisibility and the backflow of information for the system dynamics. Second, it showed explicitly that the BLP and RHP measures generally do not coincide. It demonstrated more clearly the previous result: The backflow of information must lead to the indivisibility of dynamics, but the reverse is not true.

When the nonsecular terms are included, we have investigated numerically the non-Markovian properties of the system dynamics by assuming that the environment spectrum is Lorentzian. By compared with the result under RWA, we found that the BLP measure is corrected appropriately, but the RHP measure is inconsistent with practice, showing that the RHP measure has finite applicable range.

Finally, we have discussed the complete positivity of the underlying dynamics. We have presented the sufficient and necessary conditions of the complete positivity. Numerical simulation showed that these conditions can be satisfied in the short non-Markovian time scale.

The measure of non-Markovianity is a fundamental problem in the study of open quantum system dynamics. Although several measures of non-Markovianity have been presented already, it is noted that these measures are not completely equivalent to each other. Therefore, the problem for measuring the non-Markovianity of quantum processes still remains elusive and, in some sense, controversial. At present stage, it is meaningful and necessary to expose the characteristics of various measures and their relations in some concrete systems.

The investigation of a two-level system interacting with a bath of harmonic oscillators, i.e., the spin-boson model, is of particular interest in the theory of open quantum system. In the context of quantum computation, it represents a qubit coupled to an environment, which can produce dissipation and decoherence. Though in the numerical simulations we have only considered the Lorentzian environment, our analytic results adapt to other structured environments, such as the Ohmic reservoir, the photonic band-gap material [40], etc. By properly engineering the structure of the environment, one can control the non-Markovian



dynamics of the open quantum system, so as to effectively control the evolution of some interesting physical quantities, such as the quantum coherence, quantum entanglement and discord, etc. Therefore, our work will be helpful for the quantum information processing.

Of course, our model is not fully general. First of all, we have considered only a two-level system weakly coupled a zero-temperature environment. Next, our starting point is based on the dipole interaction Hamiltonian between the atom and its environment, not on the canonical Hamiltonian. Finally, we have used the TCL perturbation expansion for the derivation of master equation eq.(2). Thus our results are still conditional and further investigations may be necessary.

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## Appendix A: Derivation of the master equation and the time-dependent forth-order coefficients

In our study, the derivation of the forth-order TCL master equation (2) is very cumbersome. Here we can present only the main clue about the deduction. Our calculation is based on the description of reference [4] about the TCL projection operator technique. By assuming a factoring initial condition  $\rho(0) = \rho_S(0) \otimes \rho_B$  for the system and environment, one obtains a homogeneous TCL master equation [see (9.33) of [4]]

$$\frac{\partial}{\partial t} \mathcal{P}\rho(t) = \mathcal{K}(t)\mathcal{P}\rho(t). \quad (\text{A1})$$

Due to the assumption of vacuum reference state  $\rho_B = |0\rangle\langle 0|$  for the environment, the TCL generator  $\mathcal{K}(t)$  only has even-order terms in its perturbation expansion. The second- and forth-order TCL generators may be calculated directly via eqs.(9.61)-(9.62) of reference [4], where the related operators  $F_k$  and  $Q_k$  in the interaction picture are given by,

$$F_k(t) = \sigma_+ e^{i\omega_0 t} + \sigma_- e^{-i\omega_0 t}, \quad (\text{A2})$$

$$Q_k(t) = g_k(b_k e^{-i\omega_k t} + b_k^+ e^{i\omega_k t}). \quad (\text{A3})$$

Calculating the second- and forth-order TCL generators and sorting them in operators, then eq.(A1) reduces to the required master equation.

In the master equation (2), each of the time-dependent coefficients consists of in principle two parts—the second and the forth order parts. The second-order parts have relatively simple expressions, but the expressions of the forth-order parts are very complex. In terms of abbreviation  $t_{ij} = t_i - t_j$  with  $t_0 \equiv t$ ,  $C(t) = \int d\omega J(\omega) \cos \omega t$ ,  $S(t) = \int d\omega J(\omega) \sin \omega t$  and  $\mathbb{T} \int = \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3$ , the forth-order coefficients may be written in the following,

$$\begin{aligned} S_+^{IV}(t) = 2\mathbb{T} \int \{ & [S(t_{02}) \sin(\omega_0 t_{03}) - 3C(t_{02}) \cos(\omega_0 t_{03})] C(t_{13}) \sin(\omega_0 t_{12}) \\ & + [C(t_{02}) \sin(\omega_0 t_{03}) - S(t_{02}) \cos(\omega_0 t_{03})] S(t_{13}) \sin(\omega_0 t_{12}) \\ & + [S(t_{03}) \sin(\omega_0 t_{02}) - 3C(t_{03}) \cos(\omega_0 t_{02})] C(t_{12}) \sin(\omega_0 t_{13}) \\ & + [C(t_{03}) \sin(\omega_0 t_{02}) - S(t_{03}) \cos(\omega_0 t_{02})] S(t_{12}) \sin(\omega_0 t_{13}) \\ & + [-S(t_{03}) \sin(\omega_0 t_{01}) - C(t_{03}) \cos(\omega_0 t_{01})] C(t_{12}) \sin(\omega_0 t_{23}) \\ & + [-C(t_{03}) \sin(\omega_0 t_{01}) + S(t_{03}) \cos(\omega_0 t_{01})] S(t_{12}) \sin(\omega_0 t_{23}) \}, \end{aligned} \quad (\text{A4})$$

$$\begin{aligned} S_-^{IV}(t) = 2\mathbb{T} \int \{ & [S(t_{02}) \sin(\omega_0 t_{03}) + C(t_{02}) \cos(\omega_0 t_{03})] C(t_{13}) \sin(\omega_0 t_{12}) \\ & + [C(t_{02}) \sin(\omega_0 t_{03}) - S(t_{02}) \cos(\omega_0 t_{03})] S(t_{13}) \sin(\omega_0 t_{12}) \\ & + [S(t_{03}) \sin(\omega_0 t_{02}) + C(t_{03}) \cos(\omega_0 t_{02})] C(t_{12}) \sin(\omega_0 t_{13}) \\ & + [C(t_{03}) \sin(\omega_0 t_{02}) - S(t_{03}) \cos(\omega_0 t_{02})] S(t_{12}) \sin(\omega_0 t_{13}) \\ & + [-S(t_{03}) \sin(\omega_0 t_{01}) - C(t_{03}) \cos(\omega_0 t_{01})] C(t_{12}) \sin(\omega_0 t_{23}) \\ & + [-C(t_{03}) \sin(\omega_0 t_{01}) + S(t_{03}) \cos(\omega_0 t_{01})] S(t_{12}) \sin(\omega_0 t_{23}) \}, \end{aligned} \quad (\text{A5})$$

$$\begin{aligned} \Gamma_{\pm}^{IV}(t) = -8\mathbb{T} \int \{ & [C(t_{13}) \sin(\omega_0 t_{03}) \pm S(t_{13}) \cos(\omega_0 t_{03})] C(t_{02}) \sin(\omega_0 t_{12}) \\ & + [C(t_{12}) \sin(\omega_0 t_{02}) \pm S(t_{12}) \cos(\omega_0 t_{02})] C(t_{03}) \sin(\omega_0 t_{13}) \\ & \mp [S(t_{03}) C(t_{12}) + C(t_{03}) S(t_{12})] \sin(\omega_0 t_{23}) \cos(\omega_0 t_{01}) \}, \end{aligned} \quad (\text{A6})$$

$$\Gamma_0(t) = 16\mathbb{T} \int \{ [C(t_{02}) C(t_{13}) + S(t_{02}) S(t_{13})] \sin(\omega_0 t_{03}) \sin(\omega_0 t_{12}) \} \quad (\text{A7})$$

$$\begin{aligned}
& + [C(t_{03})C(t_{12}) + S(t_{03})S(t_{12})] \sin(\omega_0 t_{02}) \sin(\omega_0 t_{13}) \\
& + [C(t_{03})C(t_{12}) - S(t_{03})S(t_{12})] \sin(\omega_0 t_{01}) \sin(\omega_0 t_{23}) \},
\end{aligned}$$

$$\begin{aligned}
\alpha^{IV}(t) = & -8T \int \{ S(t+t_2)S(t_{13}) \sin \omega_0(t+t_3) \sin(\omega_0 t_{12}) \\
& + S(t+t_3)S(t_{12}) \sin \omega_0(t+t_2) \sin(\omega_0 t_{13}) \\
& + [C(t_{03})C(t_{12}) - S(t_{03})S(t_{12})] \sin \omega_0(t+t_1) \sin(\omega_0 t_{23}) \},
\end{aligned} \tag{A8}$$

$$\begin{aligned}
\beta^{IV}(t) = & 8T \int \{ S(t_{02})S(t_{13}) \cos \omega_0(t+t_3) \sin(\omega_0 t_{12}) \\
& + S(t_{03})S(t_{12}) \cos \omega_0(t+t_2) \sin(\omega_0 t_{13}) \\
& + [C(t_{03})C(t_{12}) - S(t_{03})S(t_{12})] \cos \omega_0(t+t_1) \sin(\omega_0 t_{23}) \}.
\end{aligned} \tag{A9}$$

## Appendix B: Derivation of Bloch equation

According to the definition of Bloch vector  $b_j(t) = \text{Tr}[\rho(t)\sigma_j]$ , we have  $\dot{b}_j(t) = \text{Tr}[\dot{\rho}(t)\sigma_j]$ . By inserting master equation (2) into it and after some deduction, one can obtain the required Bloch equation. For example, for the component equation concerning  $\dot{b}_x$  we have,

$$\dot{b}_x(t) = -i\text{Tr}\{[H_{LS}(t), \rho(t)]\sigma_x\} + \text{Tr}\{D[\rho(t)]\sigma_x\} + \text{Tr}\{D'[\rho(t)]\sigma_x\}. \tag{B1}$$

By use of the circulation property of trace operation and the Pauli algorithm, one easily get  $-i\text{Tr}\{[H_{LS}(t), \rho(t)]\sigma_x\} = (S_- - S_+)b_y$ ,  $\text{Tr}\{D[\rho(t)]\sigma_x\} = -\frac{1}{2}(\Gamma_- + \Gamma_+ + \Gamma_0)b_x$ , and  $\text{Tr}\{D'[\rho(t)]\sigma_x\} = \alpha b_x - \beta b_y$ . Summing up them, we thus obtain eq.(21).

The Bloch eqs.(21)-(23) can also be written as the compact vector form,  $\dot{\mathbf{b}} = M\mathbf{b} + \mathbf{v}$ , with the damping matrix  $M$  and drift matrix  $\mathbf{v}$  given respectively by

$$M = \begin{pmatrix} -\frac{1}{2}(\Gamma_- + \Gamma_+ + \Gamma_0 - 2\alpha) & S_- - S_+ - \beta & 0 \\ -(S_- - S_+ + \beta) & -\frac{1}{2}(\Gamma_- + \Gamma_+ + \Gamma_0 + 2\alpha) & 0 \\ 0 & 0 & -(\Gamma_- + \Gamma_+) \end{pmatrix}, \tag{B2}$$

and  $\mathbf{v}^T = \left( 0, 0, \Gamma_+ - \Gamma_- \right)$ . Note that the damping matrix is in block diagonal form.

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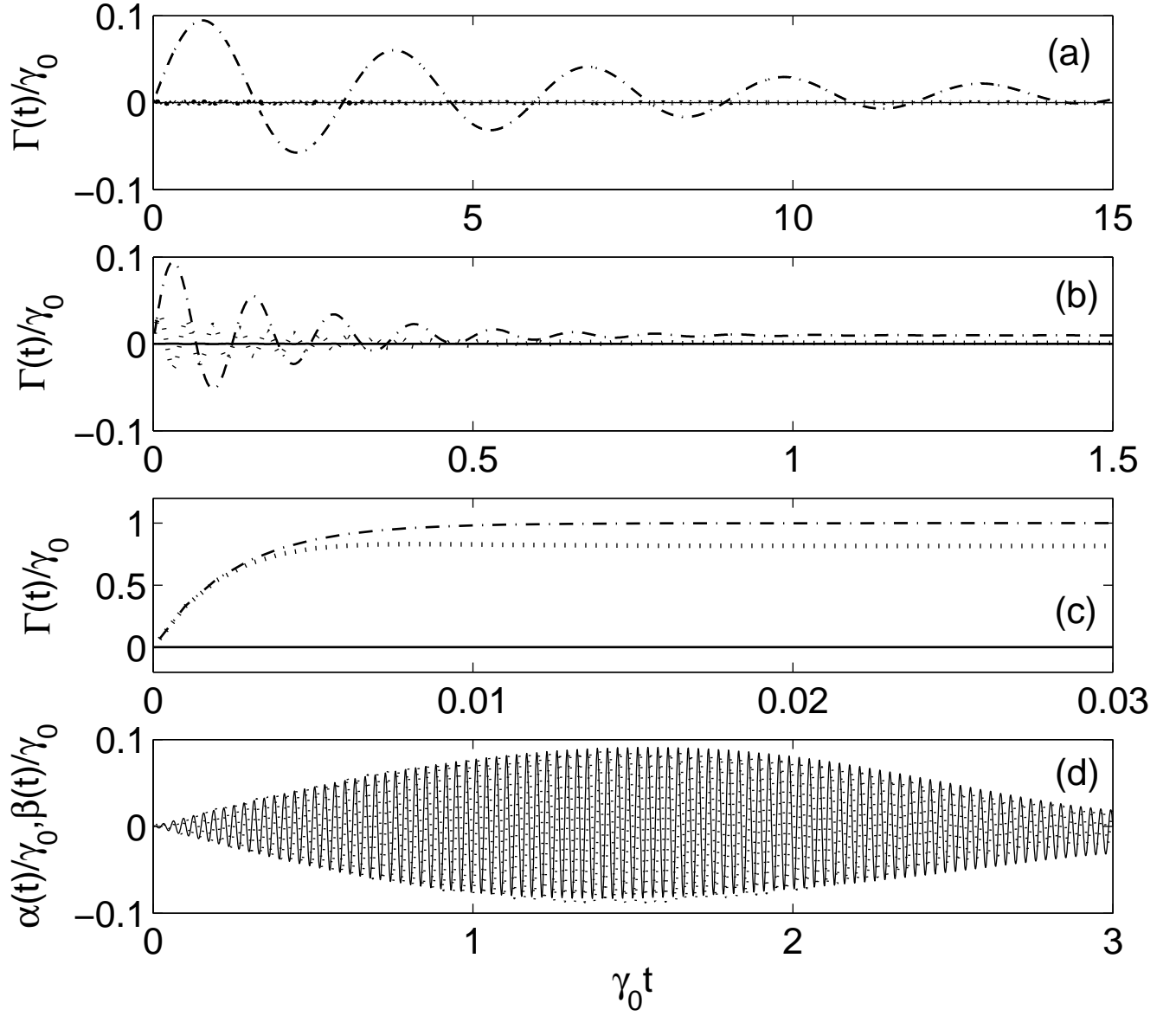


FIG. 1. Evolution of the time-dependent coefficients. The dot-dash line, dot line and solid line in (a),(b) and (c) correspond to respectively the evolutions of  $\Gamma_-$ ,  $\Gamma_+$  and  $\Gamma_0$ , while the solid and dot lines in (d) refer to the evolutions of  $\alpha$  and  $\beta$ . Where we choose  $\omega_0 = 100\gamma_0$ , and  $\lambda = 0.2\gamma_0$ ,  $\Delta = 2\gamma_0$  for (a);  $\lambda = 5\gamma_0$ ,  $\Delta = 50\gamma_0$  for (b);  $\lambda = 400\gamma_0$ ,  $\Delta = 10\gamma_0$  for (c). The parameters for (d) are the same as that of (a).

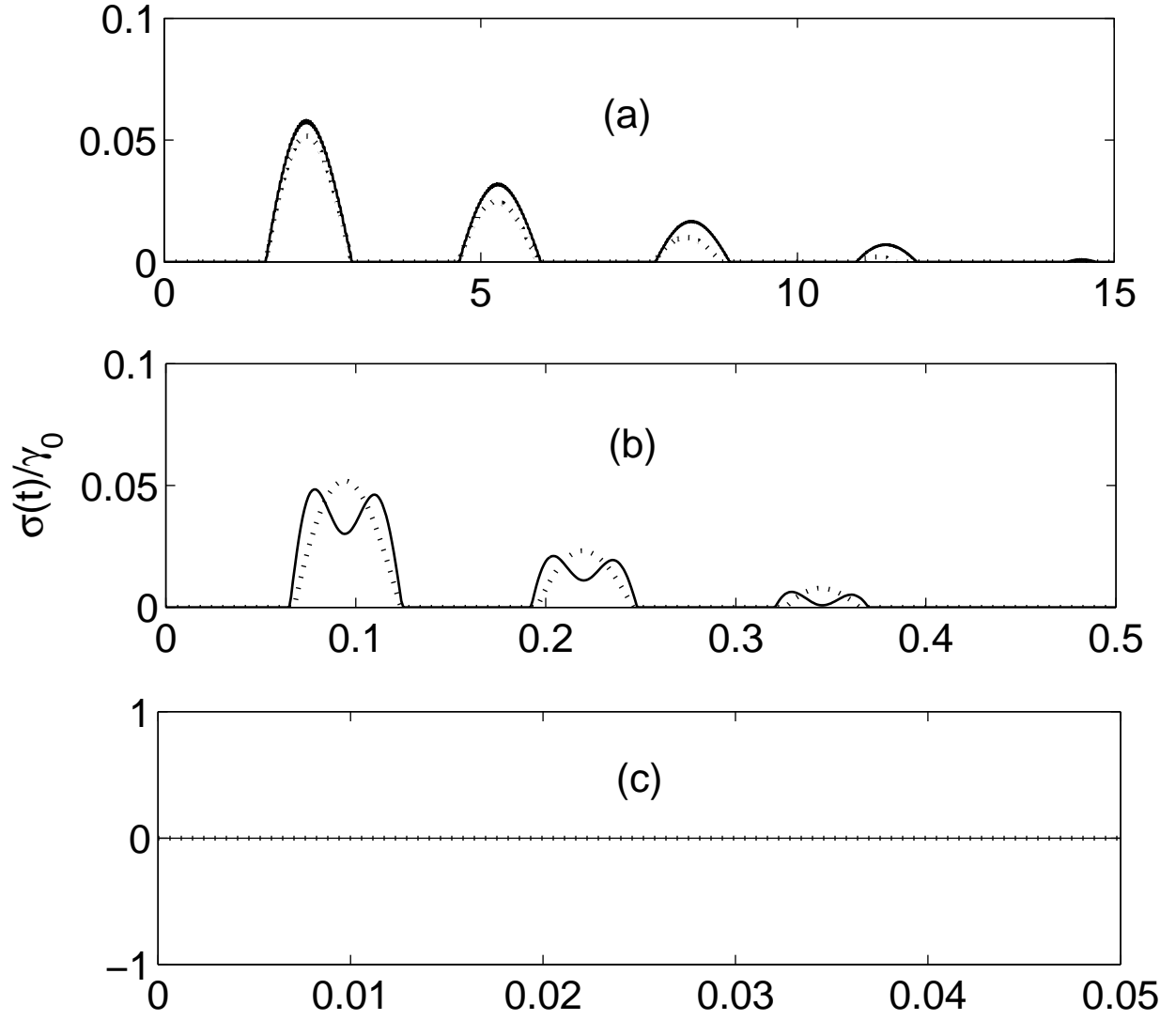


FIG. 2. Time evolution of  $\sigma(t)$ , with the solid and dot lines corresponding to respectively eqs.(25) and (39). The parameters in (a),(b) and (c) are set to be in accordance with that in Fig.1.

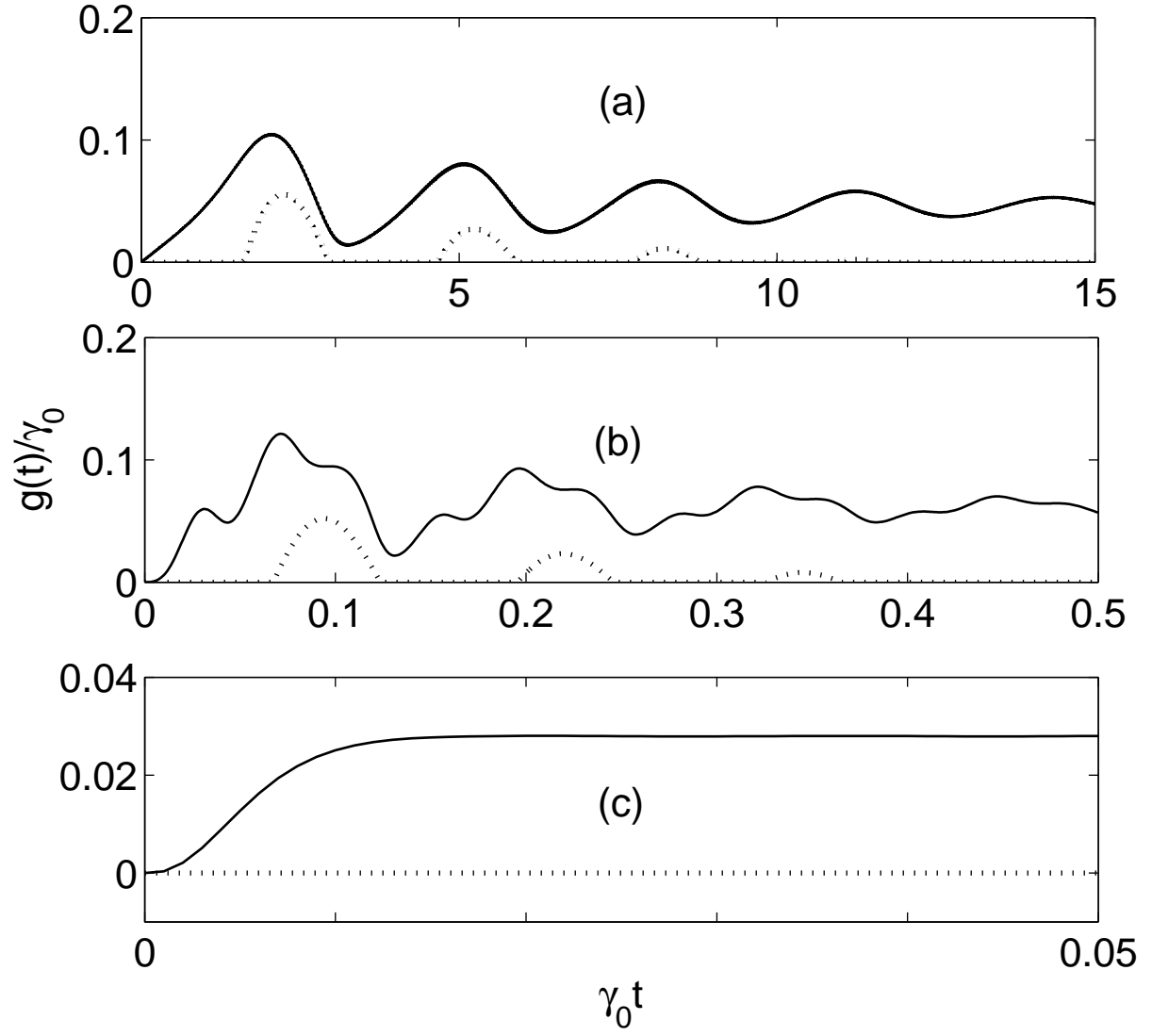


FIG. 3. Time evolution of  $g(t)$ , where the solid and dot lines are plotted according to eqs.(18) and (38) respectively. The parameters are set to be the same as in Fig.1.



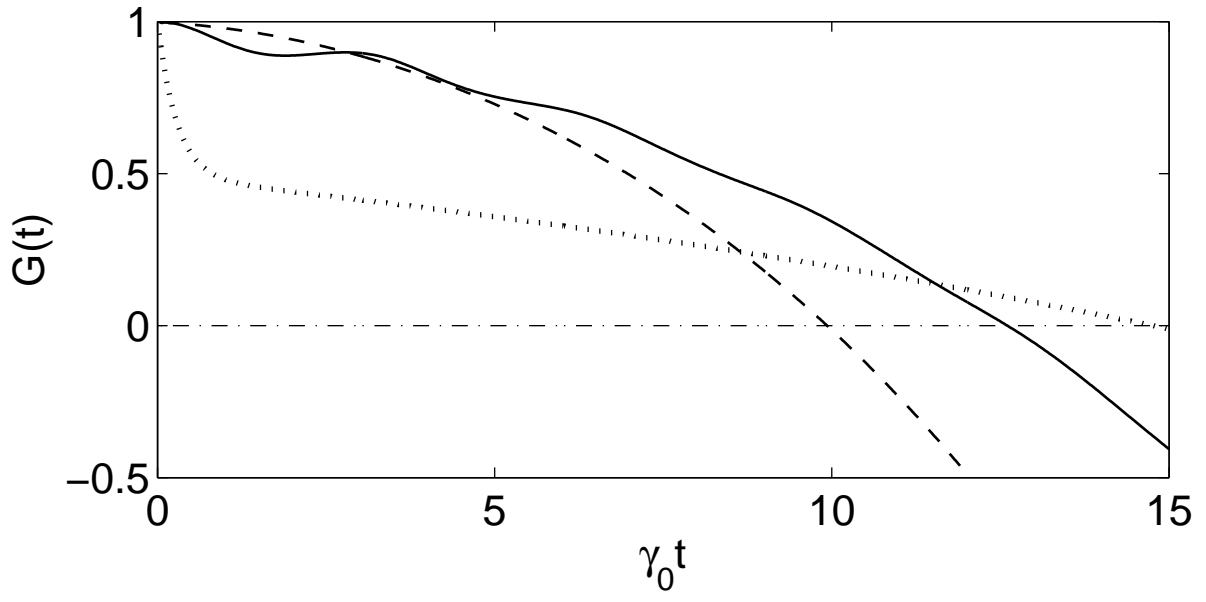


FIG. 4. Time evolution of  $G(t)$ , where the solid, dash and dot lines correspond to respectively the parameters in Fig.1 (a), (b) and (c).